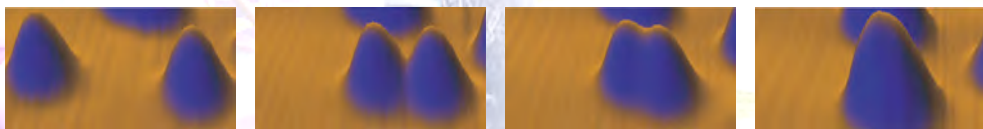


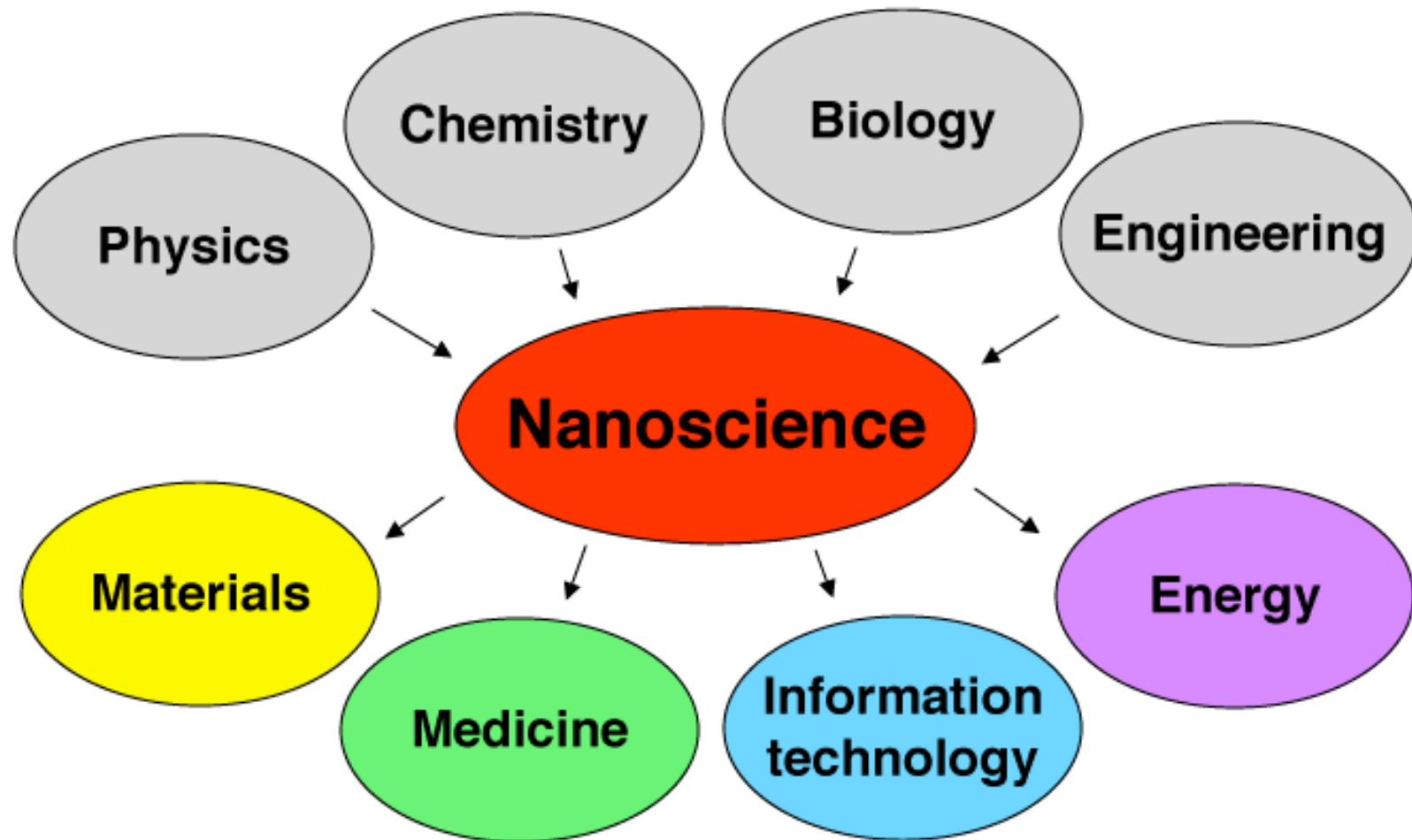
# THE MOLECULAR FOUNDRY

**A DOE User Facility  
for Nanoscale Science Research  
at Lawrence Berkeley National Lab**

**Jim De Yoreo, Deputy Director for Research**



# Nanoscience: *Multidisciplinary* research with *multiple* applications



No one research group can do it all!

# Mission of the Molecular Foundry



## Purpose

**Provide nanoscience capabilities to researchers from any discipline, and any institution, to come, free of charge, to:**

- **use state-of-the-art instruments**
- **learn leading-edge techniques**
- **collaborate with experts in a wide range of nanoscience disciplines**

## Impact

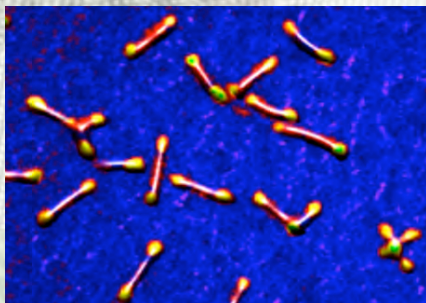
**....so that they may more effectively pursue their own research interests.**



# Six facilities, one team

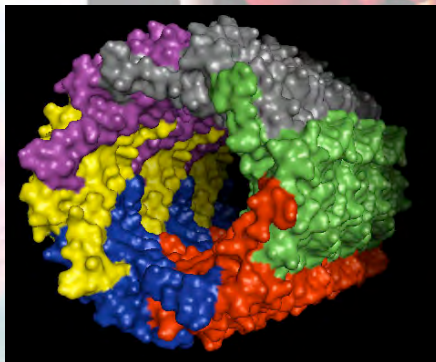
The Molecular Foundry  
A Nanostructures

## Inorganic Nanostructures



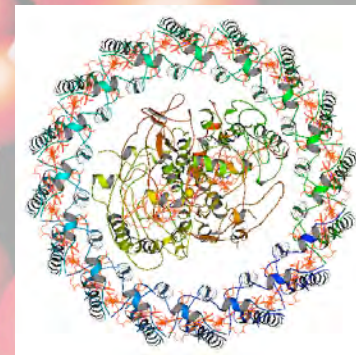
A. Paul Alivisatos

## Biological Nanostructures



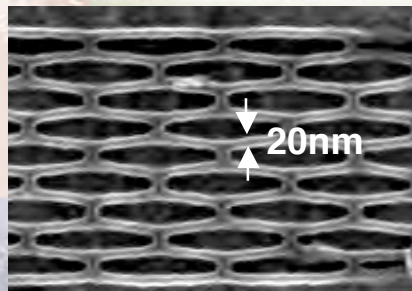
Carolyn Bertozzi

## Organic and Macromolecular Synthesis



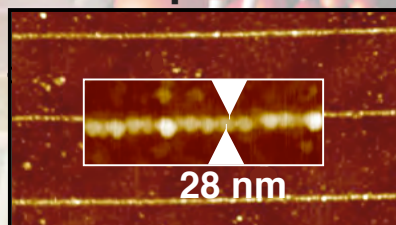
Jean Fréchet

## Nanofabrication



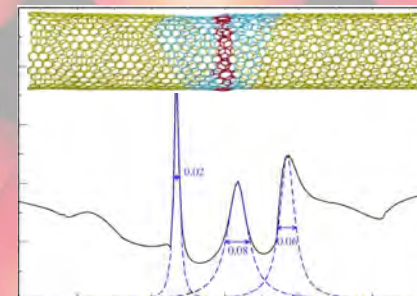
Jeffrey Bokor

## Imaging and Manipulation



Miquel Salmeron

## Theory of Nanostructures



Steven G. Louie



# PRESENT AND PROJECTED STAFF

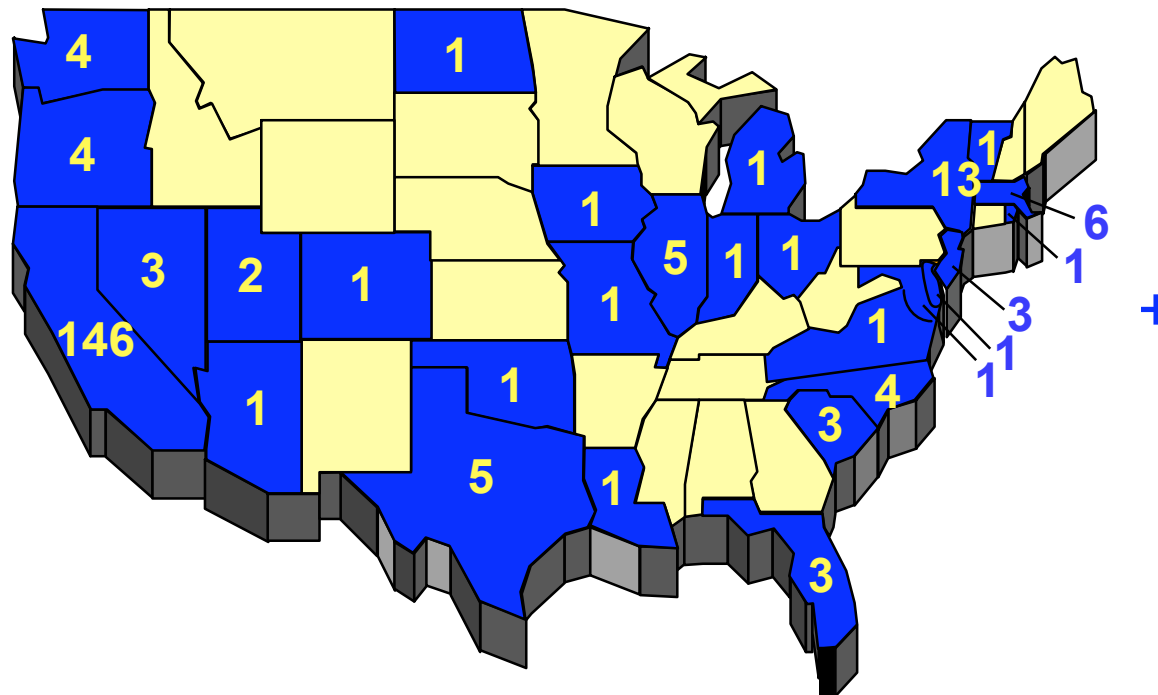


- Director and Deputy Directors
- 6 Scientific Directors
- 29 PhD Scientists (Staff Scientists and Post docs)
- 12 Technical staff (Res. Assoc. and Eng. Assoc.)
- 5 Other (User Program, Outreach, EH&S, IT, Admin.)
- **Present total = 54**
- ~ 6 positions to be filled
- **Total staff projected at steady-state = ~ 60**
- (~ 6 scientists per Facility working with Users)

# Users come from around the world



- 459 proposals received, 245 proposals accepted (~ 600 “Users”)
- Academia, Industry, National Labs
- 219 domestic, 26 international
- 28 states and 11 foreign countries represented



Australia  
Austria  
France  
Ireland  
Italy  
Germany  
Netherlands  
Spain  
South Korea  
Taiwan  
UK

# Types of Foundry User Projects



- Obtain nanostructures
- Develop new nanoscale materials/devices and methods
- Learn to use nanoscale materials and methods
- Learn to replicate new instruments/techniques
- Pursue long term collaborations
- Materials only/Instrument only
- Strategic User Partnerships (i.e., Intel)

# NSRCs must also have their own internal research program



## Purpose

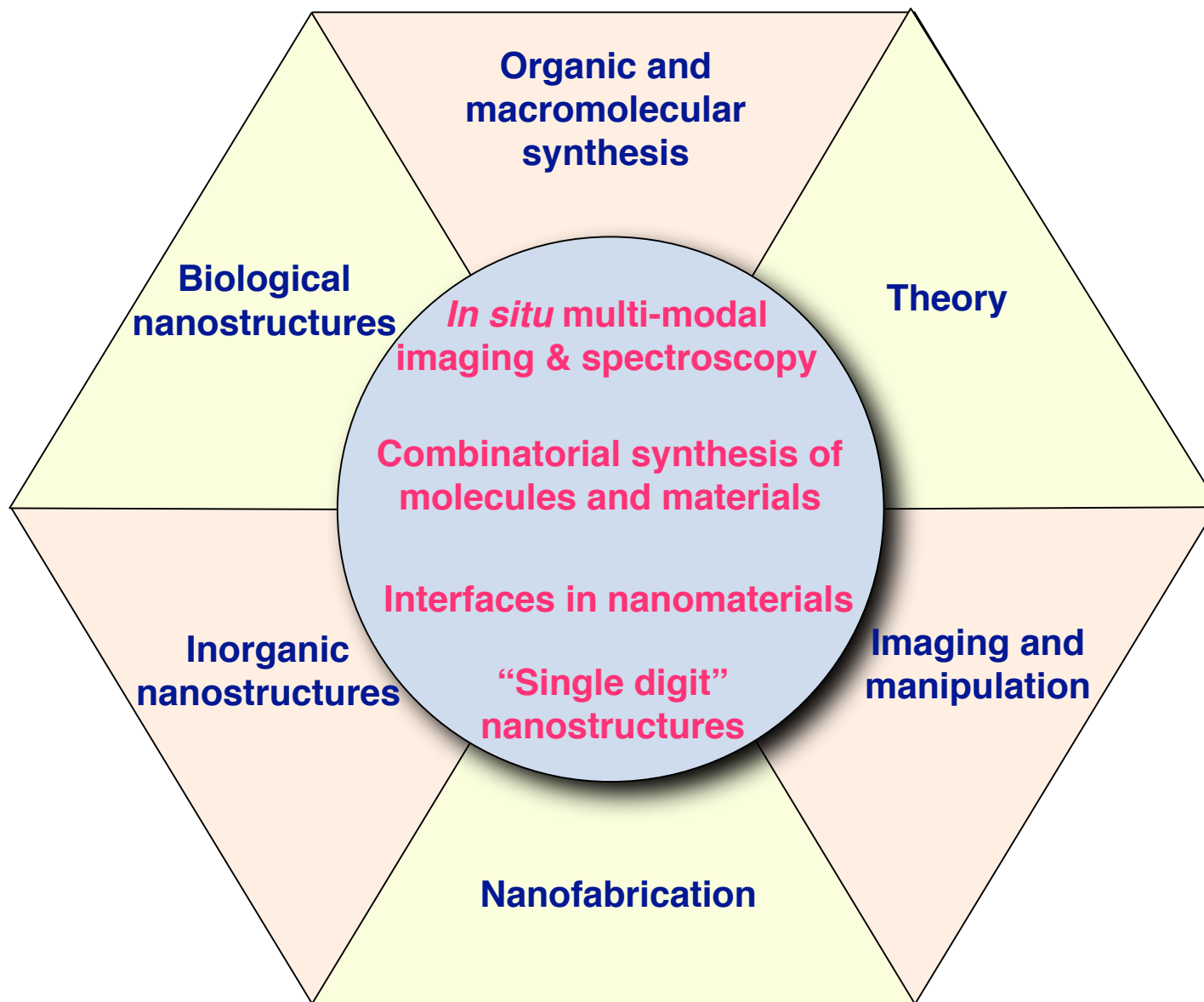
**Advance the field of nanoscience through a vibrant program of leading edge research**

## Impact

**...to provide rapid availability of most advance capabilities in nanoscience to Users**



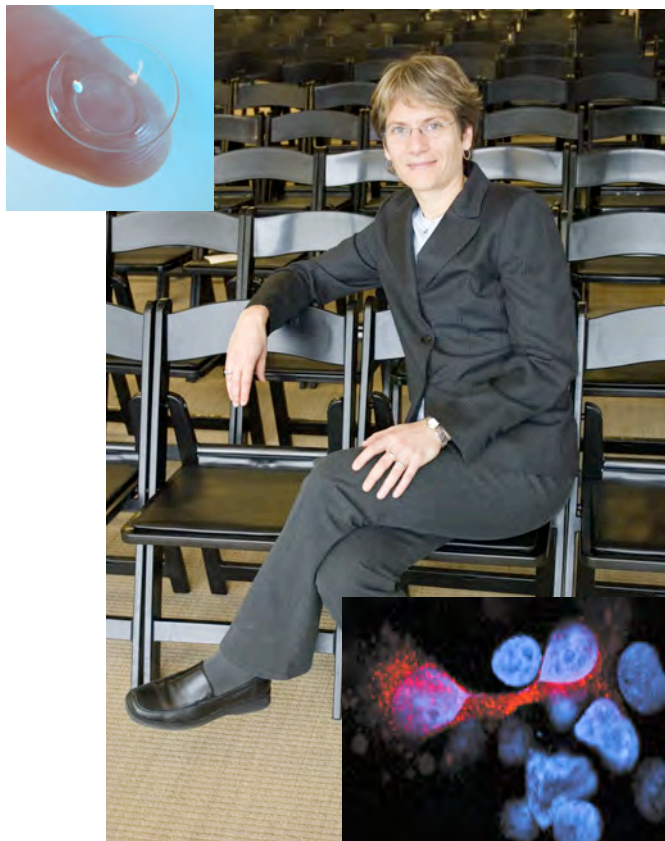
# Four research themes integrate the Foundry's six facilities



# Biological Nanostructures Facility



**Prof. Carolyn Bertozzi, Scientific Director**

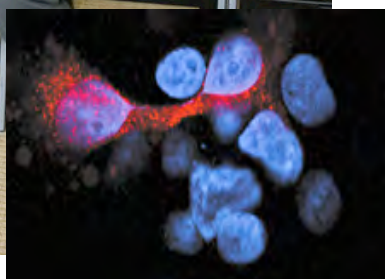


## **Expertise:**

- New nanomaterials inspired by nature
- Nanotechnologies for biological research
- Building nanomaterials from biological components

## **Current capabilities:**

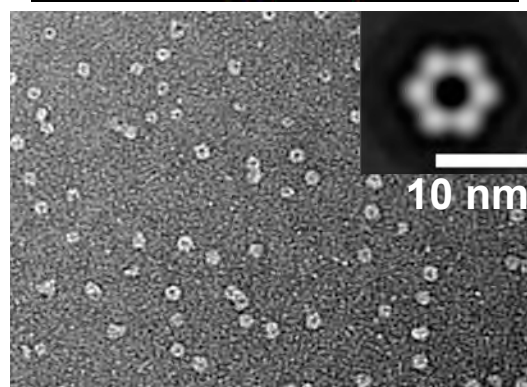
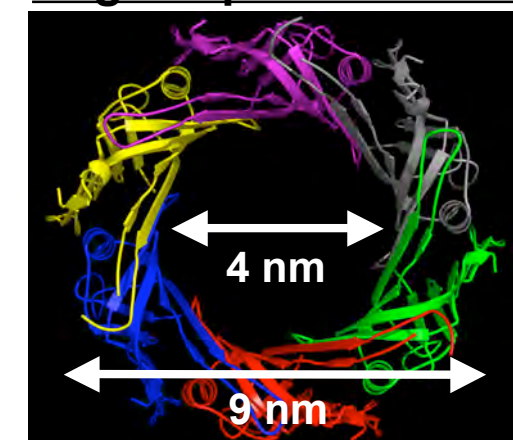
- Mammalian, plant, microbial cell culture
- Protein engineering
- RNA preparation
- Bioconjugation chemistry
- Cell immortalization via telomerase expression
- Phage display for nanocrystal-binding proteins/peptides
- Cellular components/products for bio/inorganic assemblies
- Genetic engineering of cell lines for materials integration



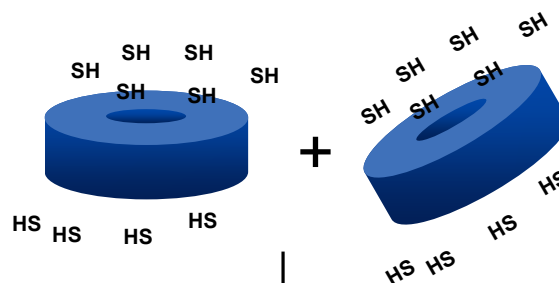
# Protein subunits as building blocks



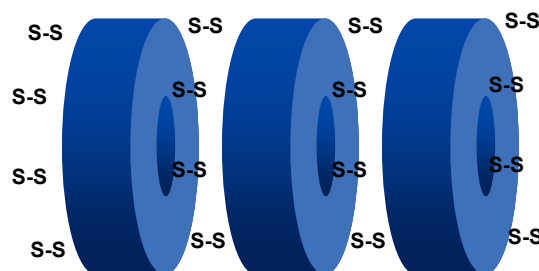
**Hcp1 protein forms a ring-shaped hexamer**



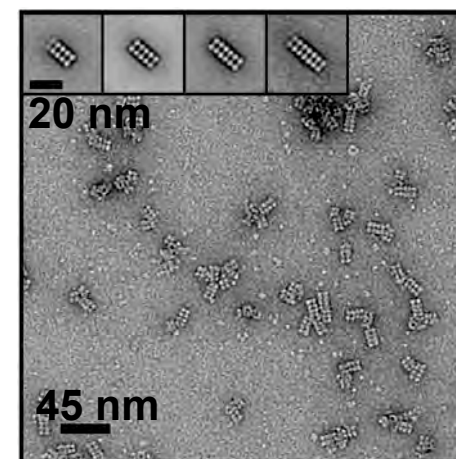
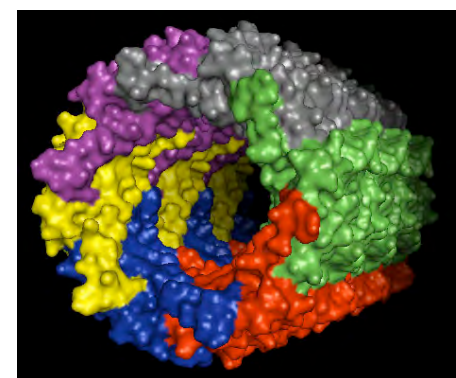
**6 cysteines were introduced into each ring face**



**Oxidation**



**Rings self-assemble into covalent nanotubes**



**Can rings be engineered to self-assemble into tubes?**

- Drug delivery
- Ion selection
- Structural scaffolds

Foundry User: Joe Mougous

Foundry Staff: Ron Zuckerman

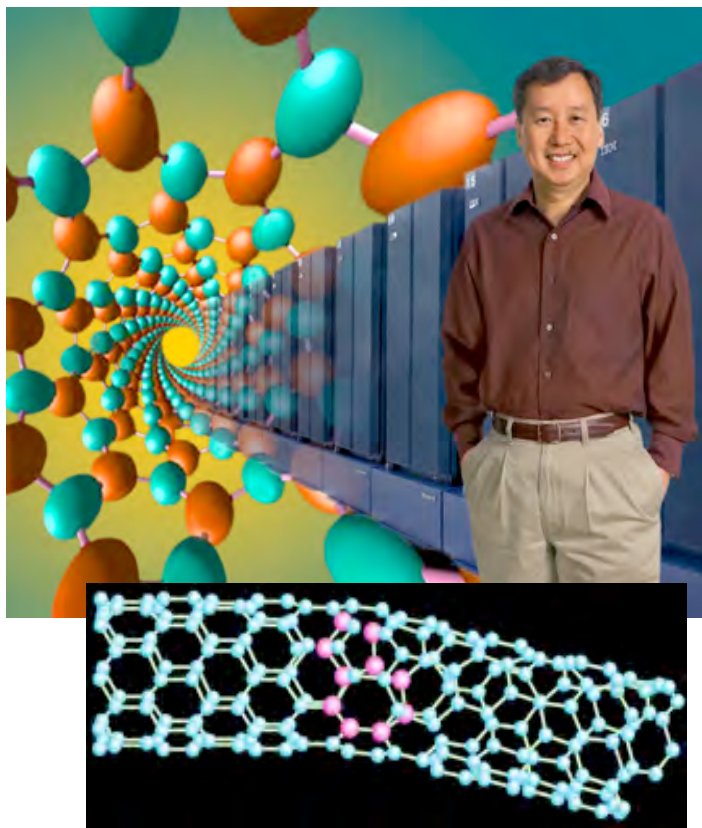
*“Single digit” nano*

Ballister et al., *PNAS* (2008)

# Theory of Nanostructures Facility



**Prof. Steven Louie, Scientific Director**



## **Expertise:**

- Electronic structure of nanomaterials and molecular junctions
- Spectroscopic prediction and interpretation
- Soft matter assembly and dynamics

## **Current capabilities:**

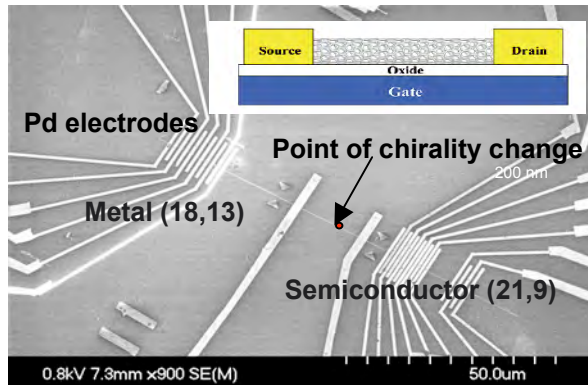
- First-principles density-functional theory
- Classical & *ab initio* molecular dynamics
- Excited-state properties with the GW/Bethe-Salpeter equation approach
- Electron transport at finite bias with a first-principles scattering-state method
- Statistical mechanical approaches



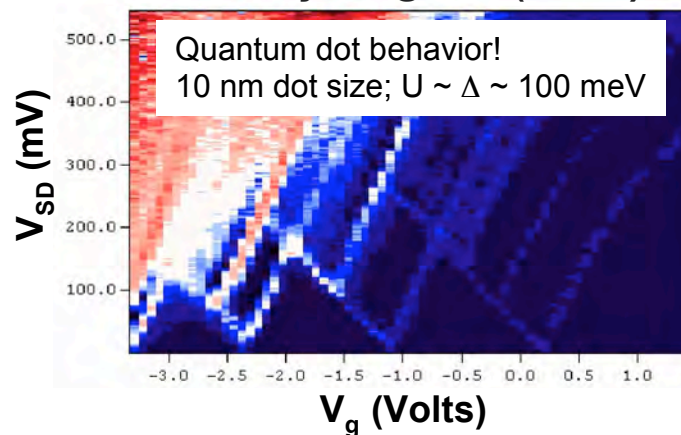
# Carbon nanotube heterojunctions



**SEM image of (18,13)-(21,9) junction**



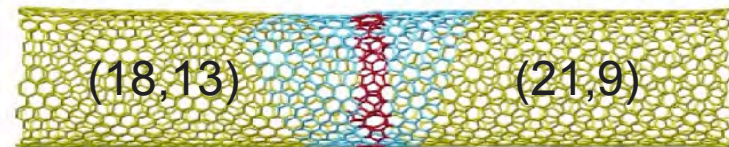
**Stability diagram (dI/dV)**



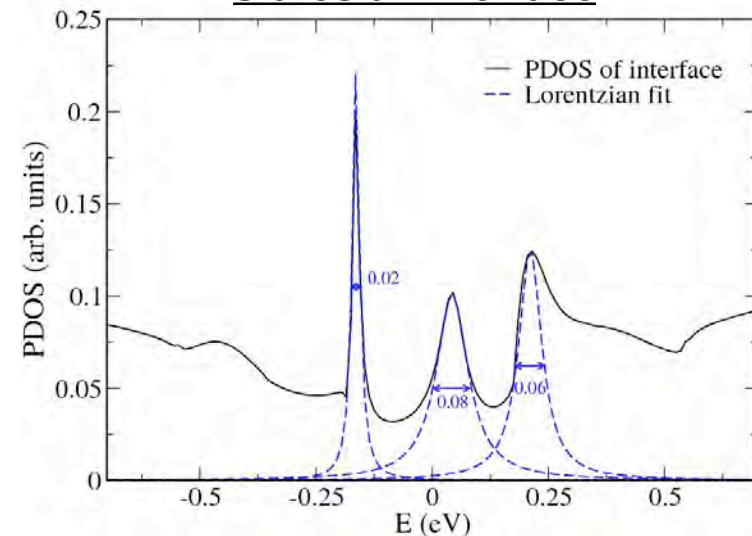
**Why do SWCNT heterojunctions show quantum dot-like behavior?**

Foundry User: Jim Hone, Columbia Univ.

**Model of SWCNT heterojunction**



**Prediction of localized states at interface**



**Defects that accommodate junction led to localized states**

Foundry Staff: J. Neaton and J. Bhattacharjee



# Imaging and Manipulation Facility



**Prof. Miquel Salmeron, Scientific Director**



## **Expertise:**

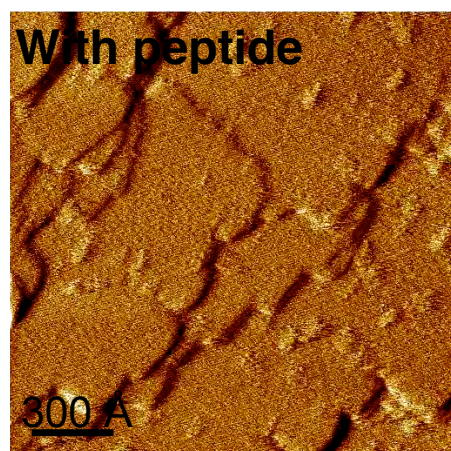
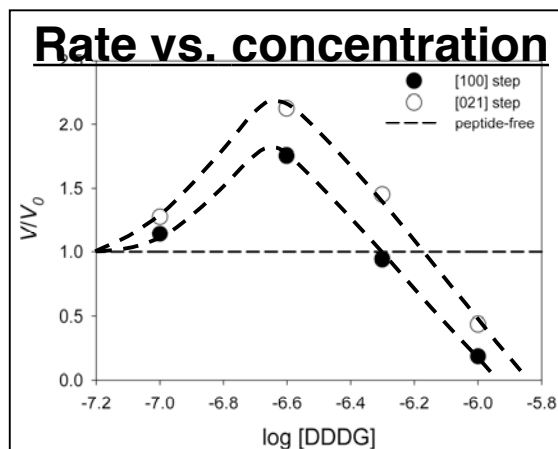
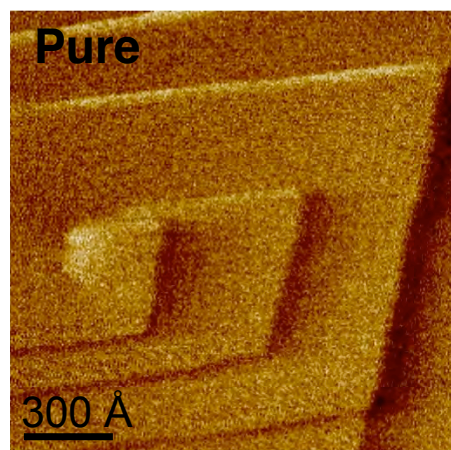
- Surface science
- In situ imaging and spectroscopy
- Molecular interactions

## **Current capabilities:**

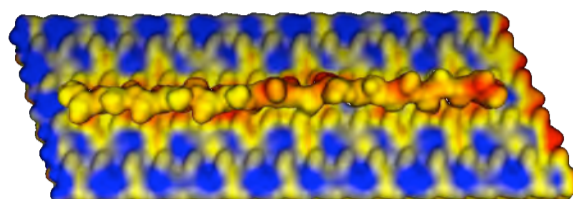
- Electron microscopy
  - 200 kV Field Emission TEM, Analytical FE-SEM, In-situ SEM, SPM and TEM
- Probe microscopy
  - Commercial multimode ambient SPM systems (air, liquids, controlled humidity, contact / non-contact)
  - Foundry-built ultra-sensitive SPM for chemical interaction work in liquids
  - UHV RT-AFM for contact imaging and electrical characterization
- Optical spectroscopy
  - Tunable ultrafast laser system (Ti:SAF / OPO), super-continuum white source, CW sources
  - Photon counters, low noise spectrometers, confocal microscope and cryostat, general optics
- Surface Analysis
  - Scanning Auger and non-monochromatic XPS
- Support
  - Optical microscopy, sample prep and chem lab

# High resolution *in situ* imaging of nanocrystal growth

## Surface morphology

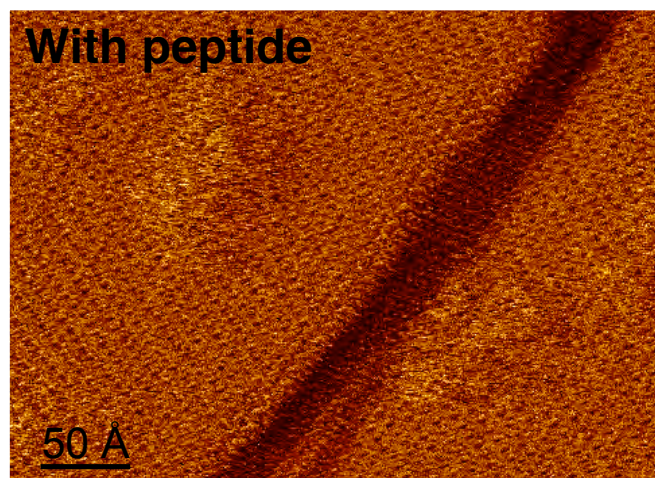
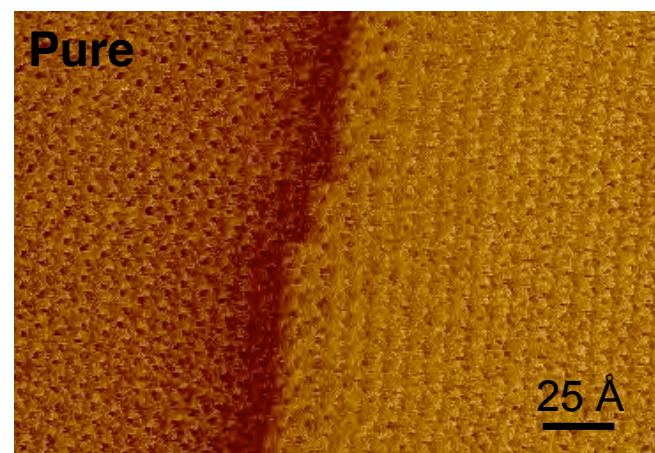


## Molecular model



How do acidic peptides modify growth of electronegative face?

## Develop atomic resolution imaging

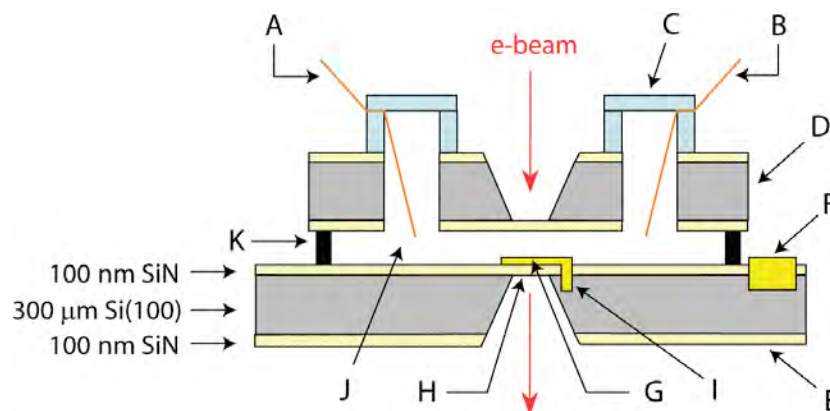
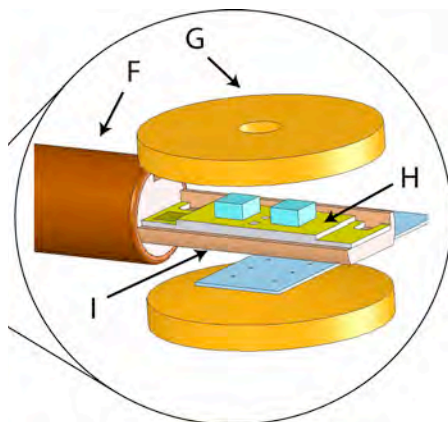


Peptides adsorb as highly charged clusters

*In situ multimodal imaging*

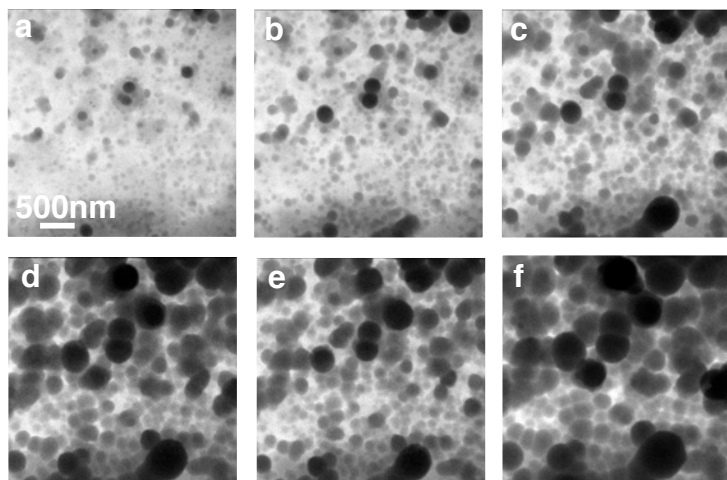


# Working with NCEM to develop fluid cells for *in situ* TEM studies of nucleation and assembly



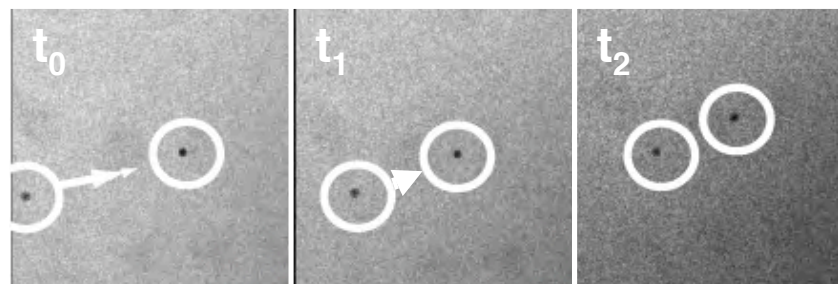
- Closed system
- Electrochemical & temperature control (0-70°C)

## Growth of silicone-based colloids



~25s intervals through 1μm cell

## Diffusion of 4nm Au nanoparticles



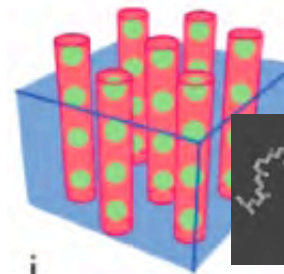
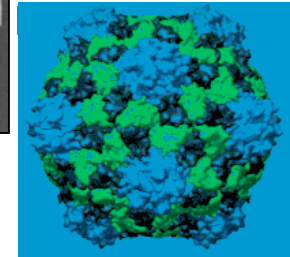
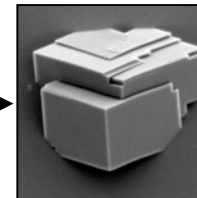
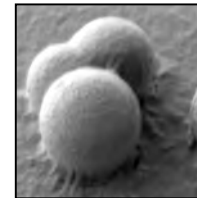
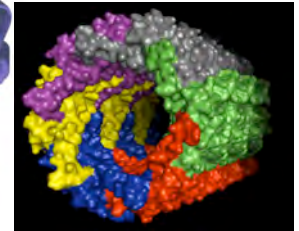
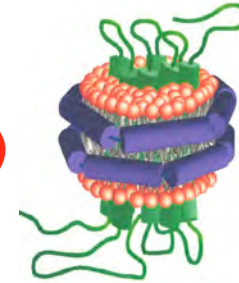
Examples illustrate ability to follow dynamics of assembly and growth

# *In situ* TEM will enable Users to probe nanomaterials assembly and reactivity



## Soft matter and organic-inorganic interfaces

- **Assembly of macromolecular complexes (Zuckerman)**
  - Protein nanotubes, Nanolipid disks
- **Bio-templated assembly (DeYoreo)**
  - Silicateins, Protein cages, Peptides
- **Supramolecular structures (Liu)**
  - Block co-polymer scaffolds



## Inorganic nanostructures

- **Catalysis at nanoparticle surfaces (Aloni, Salmeron)**
  - Photovoltaics, Solar-to-fuel catalytic structures
- **Nanowires (Mokari)**
  - Solution-liquid-solid growth

